Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 05:18 am BST

PDB ID	:	4EAR
Title	:	Crystal structure of purine nucleoside phosphorylase (W16Y, W94Y, W178Y, H257W) mutant from human complexed with DADMe-ImmG and phosphate
Authors	:	Haapalainen, A.M.; Ho, M.C.; Suarez, J.J.; Almo, S.C.; Schramm, V.L.
Deposited on	:	2012-03-22
Resolution	:	1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

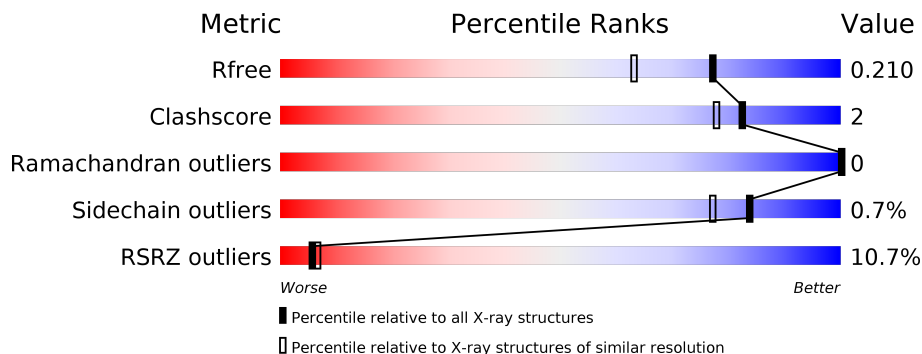|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.210
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0.7%
RSRZ outliers		10.7%

Worse   *Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	324	11% 82% 5% 13%
1	B	324	5% 85% • 11%
1	C	324	12% 82% 6% 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7404 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	283	Total 2245	C 1428	F 1	N 392	O 408	S 16	0	6	0
1	B	287	Total 2257	C 1434	F 1	N 392	O 415	S 15	0	3	0
1	C	285	Total 2248	C 1431	F 1	N 389	O 411	S 16	0	5	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	EXPRESSION TAG	UNP P00491
A	-33	ARG	-	EXPRESSION TAG	UNP P00491
A	-32	GLY	-	EXPRESSION TAG	UNP P00491
A	-31	SER	-	EXPRESSION TAG	UNP P00491
A	-30	HIS	-	EXPRESSION TAG	UNP P00491
A	-29	HIS	-	EXPRESSION TAG	UNP P00491
A	-28	HIS	-	EXPRESSION TAG	UNP P00491
A	-27	HIS	-	EXPRESSION TAG	UNP P00491
A	-26	HIS	-	EXPRESSION TAG	UNP P00491
A	-25	HIS	-	EXPRESSION TAG	UNP P00491
A	-24	GLY	-	EXPRESSION TAG	UNP P00491
A	-23	MET	-	EXPRESSION TAG	UNP P00491
A	-22	ALA	-	EXPRESSION TAG	UNP P00491
A	-21	SER	-	EXPRESSION TAG	UNP P00491
A	-20	MET	-	EXPRESSION TAG	UNP P00491
A	-19	THR	-	EXPRESSION TAG	UNP P00491
A	-18	GLY	-	EXPRESSION TAG	UNP P00491
A	-17	GLY	-	EXPRESSION TAG	UNP P00491
A	-16	GLN	-	EXPRESSION TAG	UNP P00491
A	-15	GLN	-	EXPRESSION TAG	UNP P00491
A	-14	MET	-	EXPRESSION TAG	UNP P00491
A	-13	GLY	-	EXPRESSION TAG	UNP P00491
A	-12	ARG	-	EXPRESSION TAG	UNP P00491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	ASP	-	EXPRESSION TAG	UNP P00491
A	-10	LEU	-	EXPRESSION TAG	UNP P00491
A	-9	TYR	-	EXPRESSION TAG	UNP P00491
A	-8	ASP	-	EXPRESSION TAG	UNP P00491
A	-7	ASP	-	EXPRESSION TAG	UNP P00491
A	-6	ASP	-	EXPRESSION TAG	UNP P00491
A	-5	ASP	-	EXPRESSION TAG	UNP P00491
A	-4	LYS	-	EXPRESSION TAG	UNP P00491
A	-3	ASP	-	EXPRESSION TAG	UNP P00491
A	-2	PRO	-	EXPRESSION TAG	UNP P00491
A	-1	THR	-	EXPRESSION TAG	UNP P00491
A	0	LEU	-	EXPRESSION TAG	UNP P00491
A	16	TYR	TRP	ENGINEERED MUTATION	UNP P00491
A	51	SER	GLY	ENGINEERED MUTATION	UNP P00491
A	94	TYR	TRP	ENGINEERED MUTATION	UNP P00491
A	178	TYR	TRP	ENGINEERED MUTATION	UNP P00491
A	257	FT6	HIS	ENGINEERED MUTATION	UNP P00491
B	-34	MET	-	EXPRESSION TAG	UNP P00491
B	-33	ARG	-	EXPRESSION TAG	UNP P00491
B	-32	GLY	-	EXPRESSION TAG	UNP P00491
B	-31	SER	-	EXPRESSION TAG	UNP P00491
B	-30	HIS	-	EXPRESSION TAG	UNP P00491
B	-29	HIS	-	EXPRESSION TAG	UNP P00491
B	-28	HIS	-	EXPRESSION TAG	UNP P00491
B	-27	HIS	-	EXPRESSION TAG	UNP P00491
B	-26	HIS	-	EXPRESSION TAG	UNP P00491
B	-25	HIS	-	EXPRESSION TAG	UNP P00491
B	-24	GLY	-	EXPRESSION TAG	UNP P00491
B	-23	MET	-	EXPRESSION TAG	UNP P00491
B	-22	ALA	-	EXPRESSION TAG	UNP P00491
B	-21	SER	-	EXPRESSION TAG	UNP P00491
B	-20	MET	-	EXPRESSION TAG	UNP P00491
B	-19	THR	-	EXPRESSION TAG	UNP P00491
B	-18	GLY	-	EXPRESSION TAG	UNP P00491
B	-17	GLY	-	EXPRESSION TAG	UNP P00491
B	-16	GLN	-	EXPRESSION TAG	UNP P00491
B	-15	GLN	-	EXPRESSION TAG	UNP P00491
B	-14	MET	-	EXPRESSION TAG	UNP P00491
B	-13	GLY	-	EXPRESSION TAG	UNP P00491
B	-12	ARG	-	EXPRESSION TAG	UNP P00491
B	-11	ASP	-	EXPRESSION TAG	UNP P00491
B	-10	LEU	-	EXPRESSION TAG	UNP P00491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	TYR	-	EXPRESSION TAG	UNP P00491
B	-8	ASP	-	EXPRESSION TAG	UNP P00491
B	-7	ASP	-	EXPRESSION TAG	UNP P00491
B	-6	ASP	-	EXPRESSION TAG	UNP P00491
B	-5	ASP	-	EXPRESSION TAG	UNP P00491
B	-4	LYS	-	EXPRESSION TAG	UNP P00491
B	-3	ASP	-	EXPRESSION TAG	UNP P00491
B	-2	PRO	-	EXPRESSION TAG	UNP P00491
B	-1	THR	-	EXPRESSION TAG	UNP P00491
B	0	LEU	-	EXPRESSION TAG	UNP P00491
B	16	TYR	TRP	ENGINEERED MUTATION	UNP P00491
B	51	SER	GLY	ENGINEERED MUTATION	UNP P00491
B	94	TYR	TRP	ENGINEERED MUTATION	UNP P00491
B	178	TYR	TRP	ENGINEERED MUTATION	UNP P00491
B	257	FT6	HIS	ENGINEERED MUTATION	UNP P00491
C	-34	MET	-	EXPRESSION TAG	UNP P00491
C	-33	ARG	-	EXPRESSION TAG	UNP P00491
C	-32	GLY	-	EXPRESSION TAG	UNP P00491
C	-31	SER	-	EXPRESSION TAG	UNP P00491
C	-30	HIS	-	EXPRESSION TAG	UNP P00491
C	-29	HIS	-	EXPRESSION TAG	UNP P00491
C	-28	HIS	-	EXPRESSION TAG	UNP P00491
C	-27	HIS	-	EXPRESSION TAG	UNP P00491
C	-26	HIS	-	EXPRESSION TAG	UNP P00491
C	-25	HIS	-	EXPRESSION TAG	UNP P00491
C	-24	GLY	-	EXPRESSION TAG	UNP P00491
C	-23	MET	-	EXPRESSION TAG	UNP P00491
C	-22	ALA	-	EXPRESSION TAG	UNP P00491
C	-21	SER	-	EXPRESSION TAG	UNP P00491
C	-20	MET	-	EXPRESSION TAG	UNP P00491
C	-19	THR	-	EXPRESSION TAG	UNP P00491
C	-18	GLY	-	EXPRESSION TAG	UNP P00491
C	-17	GLY	-	EXPRESSION TAG	UNP P00491
C	-16	GLN	-	EXPRESSION TAG	UNP P00491
C	-15	GLN	-	EXPRESSION TAG	UNP P00491
C	-14	MET	-	EXPRESSION TAG	UNP P00491
C	-13	GLY	-	EXPRESSION TAG	UNP P00491
C	-12	ARG	-	EXPRESSION TAG	UNP P00491
C	-11	ASP	-	EXPRESSION TAG	UNP P00491
C	-10	LEU	-	EXPRESSION TAG	UNP P00491
C	-9	TYR	-	EXPRESSION TAG	UNP P00491
C	-8	ASP	-	EXPRESSION TAG	UNP P00491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ASP	-	EXPRESSION TAG	UNP P00491
C	-6	ASP	-	EXPRESSION TAG	UNP P00491
C	-5	ASP	-	EXPRESSION TAG	UNP P00491
C	-4	LYS	-	EXPRESSION TAG	UNP P00491
C	-3	ASP	-	EXPRESSION TAG	UNP P00491
C	-2	PRO	-	EXPRESSION TAG	UNP P00491
C	-1	THR	-	EXPRESSION TAG	UNP P00491
C	0	LEU	-	EXPRESSION TAG	UNP P00491
C	16	TYR	TRP	ENGINEERED MUTATION	UNP P00491
C	51	SER	GLY	ENGINEERED MUTATION	UNP P00491
C	94	TYR	TRP	ENGINEERED MUTATION	UNP P00491
C	178	TYR	TRP	ENGINEERED MUTATION	UNP P00491
C	257	FT6	HIS	ENGINEERED MUTATION	UNP P00491

- Molecule 2 is 2-amino-7-{[(3R,4R)-3-hydroxy-4-(hydroxymethyl)pyrrolidin-1-yl]methyl}-3,5 -dihydro-4H-pyrrolo[3,2-d]pyrimidin-4-one (three-letter code: IM5) (formula: $C_{12}H_{17}N_5O_3$).
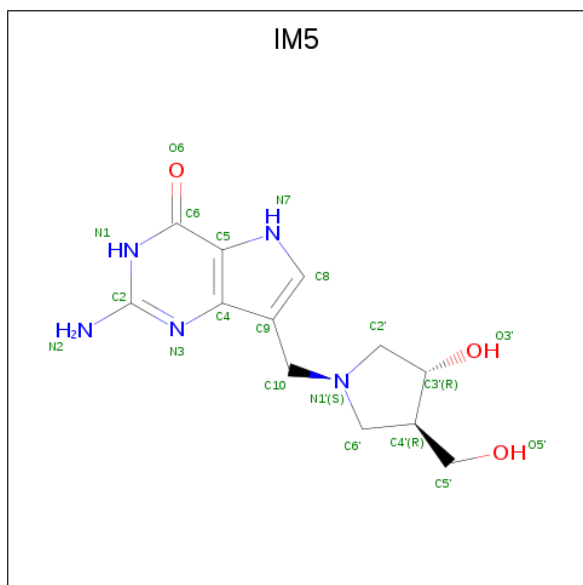
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 20	C 12	N 5	O 3	0	0
2	B	1	Total 20	C 12	N 5	O 3	0	0
2	C	1	Total 20	C 12	N 5	O 3	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4
O3

O⁻

O2 O⁻ — P = O O1

P

O⁻

O4
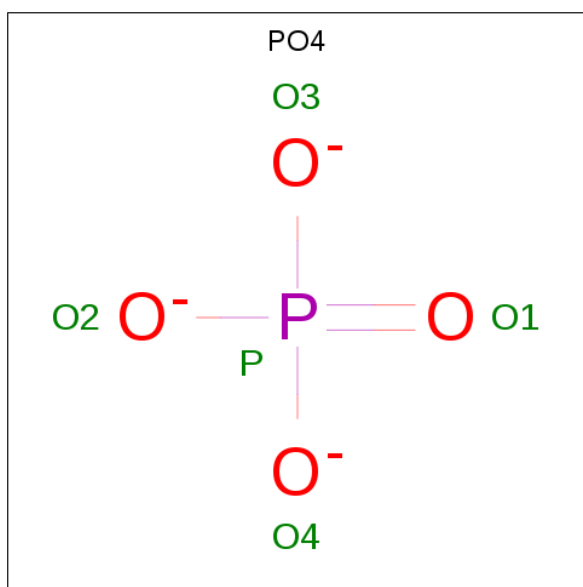
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0
3	C	1	Total 5	O 4	P 1	0	0

• Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	182	Total 184	O 184	0	2
4	B	192	Total 194	O 194	0	2
4	C	200	Total 201	O 201	0	1

W O R L D W I D E
PDB
PROTEIN DATA BANK

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
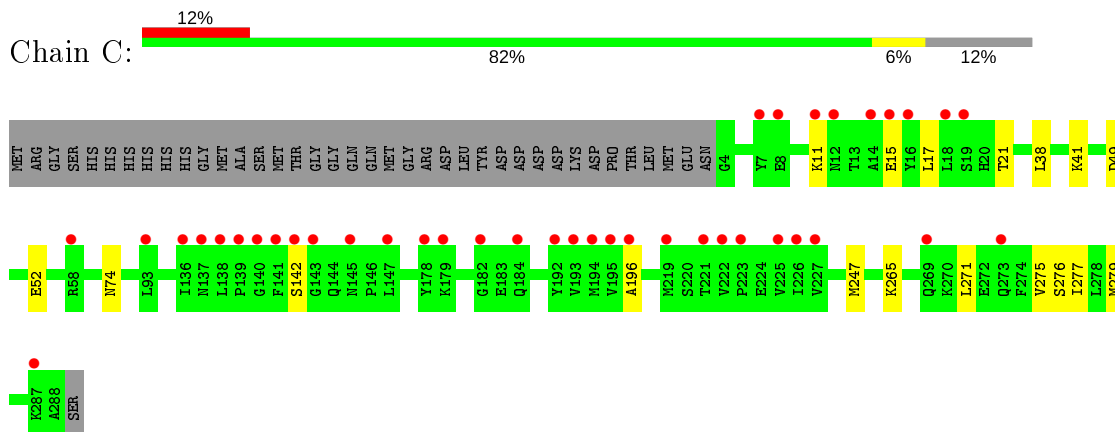
- Molecule 1: Purine nucleoside phosphorylase
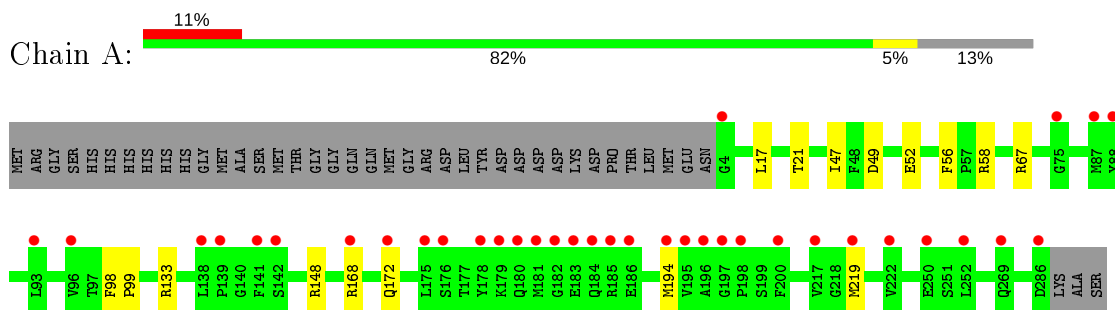
- Molecule 1: Purine nucleoside phosphorylase
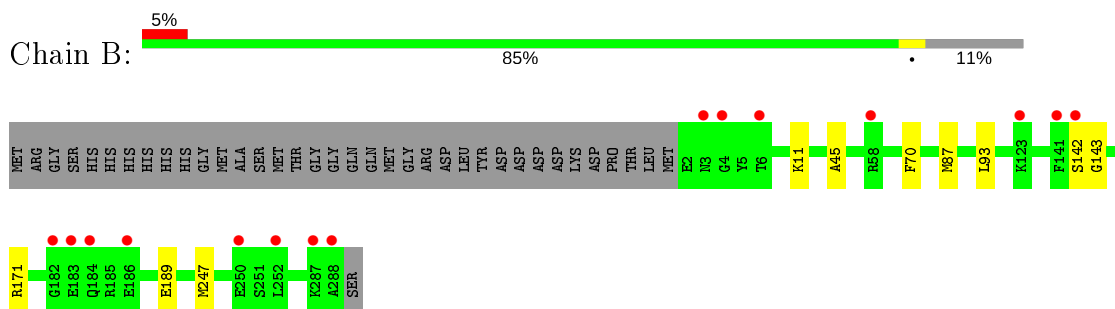
- Molecule 1: Purine nucleoside phosphorylase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.92Å　　131.10Å　　137.68Å 90.00°　　90.00°　　　90.00°	Depositor
Resolution (Å)	41.24　–　1.70 41.20　–　1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (41.24-1.70) 98.3 (41.20-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.175　,　0.203 0.184　,　0.210	Depositor DCC
R_{free} test set	5592 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 51.4	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7404	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, IM5, FT6

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.54	0/2295	0.71	0/3099
1	B	0.51	0/2298	0.70	0/3104
1	C	0.53	0/2295	0.69	0/3099
All	All	0.53	0/6888	0.70	0/9302

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2245	0	2240	11	0
1	B	2257	0	2239	14	0
1	C	2248	0	2241	11	0
2	A	20	0	17	0	0
2	B	20	0	17	0	0
2	C	20	0	17	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	184	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	194	0	0	1	0
4	C	201	0	0	1	0
All	All	7404	0	6771	34	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171[B]:ARG:HG2	1:B:171[B]:ARG:HH11	1.20	1.06
1:B:171[B]:ARG:CG	1:B:171[B]:ARG:HH11	1.75	0.99
1:A:58[A]:ARG:HG2	4:A:419:HOH:O	1.77	0.83
1:B:171[B]:ARG:HB3	1:B:171[B]:ARG:NH1	2.06	0.71
1:B:171[B]:ARG:NH1	1:B:171[B]:ARG:HG2	2.02	0.71
1:B:171[B]:ARG:CG	1:B:171[B]:ARG:NH1	2.46	0.68
1:B:171[B]:ARG:NH1	1:B:171[B]:ARG:CB	2.59	0.66
1:B:87:MET:HE2	1:B:93:LEU:HD21	1.80	0.62
1:B:171[B]:ARG:HH11	1:B:171[B]:ARG:CB	2.11	0.62
1:C:275:VAL:O	1:C:279[B]:MET:HG2	2.08	0.54
1:B:142[B]:SER:HB2	1:C:142[B]:SER:OG	2.08	0.53
1:A:133[B]:ARG:NH1	4:A:480:HOH:O	2.43	0.51
1:A:168:ARG:NH2	4:A:539:HOH:O	2.41	0.50
1:C:74:ASN:OD1	1:C:276[B]:SER:HA	2.12	0.50
1:A:148[B]:ARG:CZ	4:A:552:HOH:O	2.59	0.50
1:A:168:ARG:O	1:A:172:GLN:HG3	2.11	0.49
1:C:38:LEU:HD22	1:C:275:VAL:HG21	1.96	0.48
1:B:171[B]:ARG:HB3	1:B:171[B]:ARG:HH11	1.74	0.48
1:C:38:LEU:HD21	1:C:271:LEU:HB3	1.98	0.46
1:C:74:ASN:OD1	1:C:276[A]:SER:HA	2.17	0.45
1:A:49:ASP:O	1:A:52:GLU:HG2	2.16	0.45
1:B:247:MET:HE3	4:B:583:HOH:O	2.18	0.44
1:A:219:MET:HB2	4:A:409:HOH:O	2.18	0.43
1:A:47:ILE:HD13	1:A:67:ARG:HH21	1.83	0.43
1:B:143:GLY:HA2	1:C:196:ALA:CB	2.49	0.43
1:A:194:MET:SD	4:A:561:HOH:O	2.62	0.43
1:A:17:LEU:O	1:A:21:THR:HG22	2.19	0.42
1:C:17:LEU:O	1:C:21:THR:HG22	2.19	0.42
1:C:11:LYS:O	1:C:15:GLU:HG2	2.19	0.41
1:B:45:ALA:HA	1:B:70:PHE:O	2.20	0.41
1:C:247:MET:HE3	4:C:589:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ASP:O	1:C:52:GLU:HG2	2.21	0.41
1:A:98:PHE:HB3	1:A:99:PRO:HD3	2.03	0.40
1:B:171[B]:ARG:NH1	1:B:189:GLU:OE1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/324 (88%)	282 (99%)	4 (1%)	0	100	100
1	B	287/324 (89%)	284 (99%)	3 (1%)	0	100	100
1	C	287/324 (89%)	283 (99%)	4 (1%)	0	100	100
All	All	860/972 (88%)	849 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/268 (90%)	239 (100%)	1 (0%)	91	87
1	B	240/268 (90%)	239 (100%)	1 (0%)	91	87
1	C	240/268 (90%)	237 (99%)	3 (1%)	69	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	720/804 (90%)	715 (99%)	5 (1%)	84 77

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	PHE
1	B	11	LYS
1	C	41	LYS
1	C	265	LYS
1	C	277	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	210	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains (i)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	FT6	A	257	1	14,16,17	1.41	2 (14%)	15,22,24	1.38	4 (26%)
1	FT6	B	257	1	14,16,17	1.39	2 (14%)	15,22,24	1.41	3 (20%)
1	FT6	C	257	1	14,16,17	1.33	1 (7%)	15,22,24	1.49	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FT6	A	257	1	-	0/4/6/8	0/2/2/2
1	FT6	B	257	1	-	0/4/6/8	0/2/2/2
1	FT6	C	257	1	-	0/4/6/8	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	257	FT6	CZ2-CH2	2.82	1.40	1.36
1	A	257	FT6	CZ2-CH2	2.66	1.40	1.36
1	A	257	FT6	CD2-CE2	2.12	1.48	1.42
1	B	257	FT6	CD2-CE2	2.08	1.48	1.42
1	C	257	FT6	CZ3-CH2	2.02	1.41	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	FT6	CE3-CD2-CE2	3.12	122.30	118.17
1	C	257	FT6	CE3-CD2-CE2	3.10	122.28	118.17
1	A	257	FT6	CE3-CD2-CE2	2.52	121.51	118.17
1	B	257	FT6	CZ3-CE3-CD2	-2.50	117.65	121.13
1	C	257	FT6	CZ3-CE3-CD2	-2.43	117.75	121.13
1	C	257	FT6	CZ2-CE2-CD2	-2.36	118.13	121.16
1	B	257	FT6	CZ2-CE2-CD2	-2.31	118.18	121.16
1	A	257	FT6	CZ3-CE3-CD2	-2.30	117.94	121.13
1	A	257	FT6	CE3-CZ3-CH2	2.18	121.24	118.74
1	A	257	FT6	CZ2-CE2-CD2	-2.06	118.51	121.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	PO4	B	302	-	4,4,4	1.18	1 (25%)	6,6,6	0.88	0
3	PO4	C	302	-	4,4,4	1.47	1 (25%)	6,6,6	1.41	2 (33%)
2	IM5	A	301	-	19,22,22	1.90	6 (31%)	17,32,32	2.08	5 (29%)
3	PO4	A	302	-	4,4,4	1.30	0	6,6,6	0.97	0
2	IM5	C	301	-	19,22,22	1.60	5 (26%)	17,32,32	2.60	8 (47%)
2	IM5	B	301	-	19,22,22	1.80	4 (21%)	17,32,32	2.13	6 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IM5	A	301	-	-	0/5/18/18	0/3/3/3
2	IM5	C	301	-	-	1/5/18/18	0/3/3/3
2	IM5	B	301	-	-	0/5/18/18	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	IM5	C2-N1	4.96	1.44	1.35
2	A	301	IM5	C6'-C4'	3.82	1.58	1.52
2	B	301	IM5	C6-C5	-3.48	1.35	1.41
2	A	301	IM5	C6-N1	3.45	1.39	1.33
2	A	301	IM5	C2-N1	3.19	1.41	1.35
2	C	301	IM5	C2-N1	3.18	1.41	1.35
2	B	301	IM5	C6-N1	3.17	1.38	1.33
2	C	301	IM5	C6-C5	-2.81	1.36	1.41
2	A	301	IM5	C2'-C3'	2.80	1.56	1.52
2	C	301	IM5	C2'-C3'	2.65	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	IM5	C6-C5	-2.52	1.37	1.41
2	A	301	IM5	C10-N1'	2.35	1.52	1.47
2	B	301	IM5	O3'-C3'	2.31	1.48	1.43
2	C	301	IM5	C10-N1'	2.15	1.51	1.47
3	C	302	PO4	P-O4	-2.14	1.48	1.54
2	C	301	IM5	C6-N1	2.10	1.36	1.33
3	B	302	PO4	P-O2	-2.00	1.48	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	IM5	N3-C2-N1	-5.80	119.48	127.22
2	B	301	IM5	N3-C2-N1	-5.40	120.02	127.22
2	A	301	IM5	N3-C2-N1	-5.27	120.19	127.22
2	C	301	IM5	C5-C6-N1	-4.06	117.88	123.43
2	C	301	IM5	C9-C10-N1'	3.84	119.63	114.14
2	C	301	IM5	C3'-C2'-N1'	-3.60	97.55	104.44
2	B	301	IM5	N2-C2-N3	3.58	123.63	117.79
2	A	301	IM5	C5-C6-N1	-3.49	118.65	123.43
2	C	301	IM5	C6-N1-C2	3.08	120.82	115.93
2	A	301	IM5	C3'-C2'-N1'	-2.95	98.80	104.44
2	C	301	IM5	C10-N1'-C6'	-2.82	108.48	113.27
2	C	301	IM5	C10-C9-C8	-2.69	123.28	127.48
2	A	301	IM5	N2-C2-N3	2.48	121.84	117.79
3	C	302	PO4	O4-P-O2	2.48	115.92	107.97
2	B	301	IM5	O5'-C5'-C4'	-2.46	105.70	111.36
2	A	301	IM5	C6-N1-C2	2.39	119.73	115.93
3	C	302	PO4	O3-P-O1	-2.33	102.36	110.89
2	B	301	IM5	C2-N3-C4	2.21	121.04	116.16
2	B	301	IM5	C10-N1'-C6'	2.20	117.01	113.27
2	C	301	IM5	N2-C2-N3	2.07	121.17	117.79
2	B	301	IM5	C5-C6-N1	-2.01	120.68	123.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

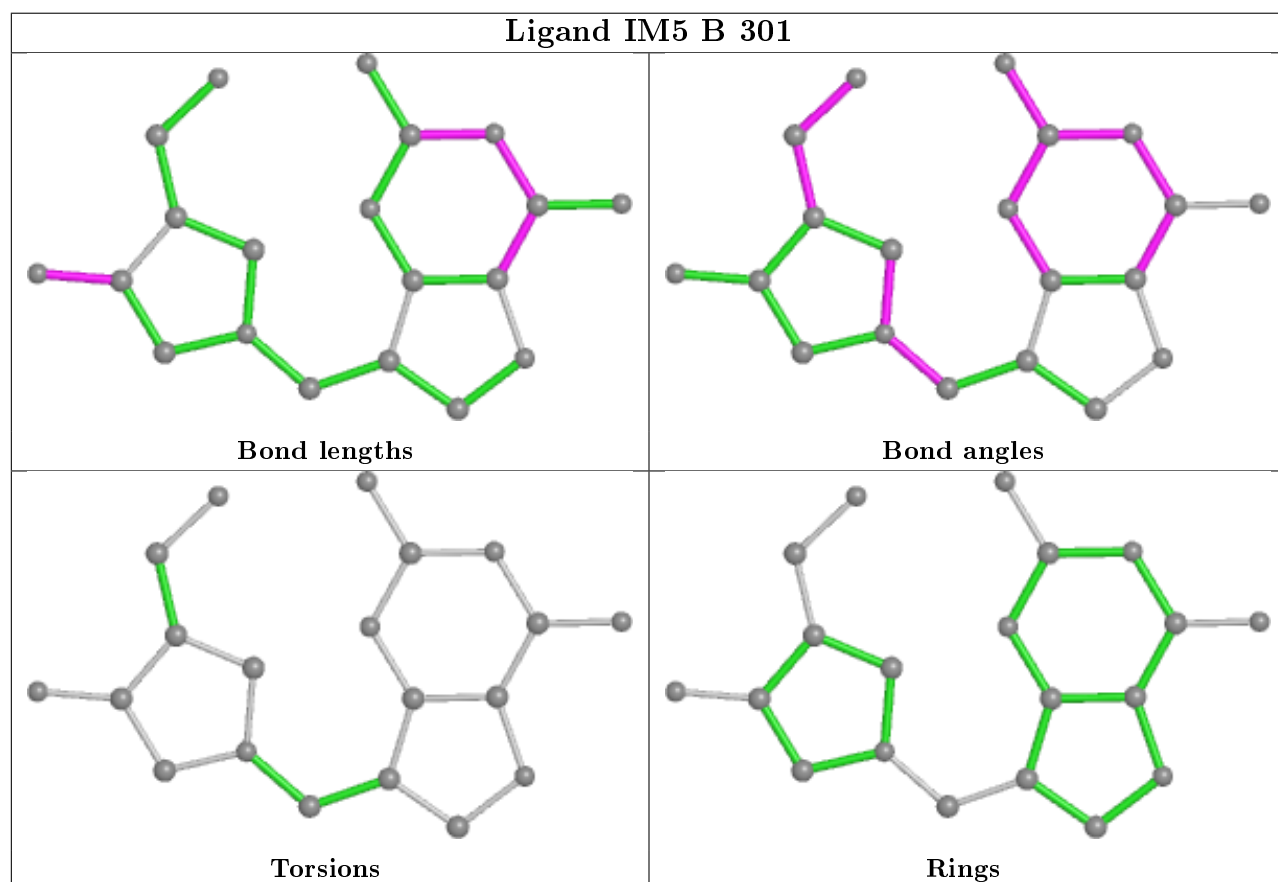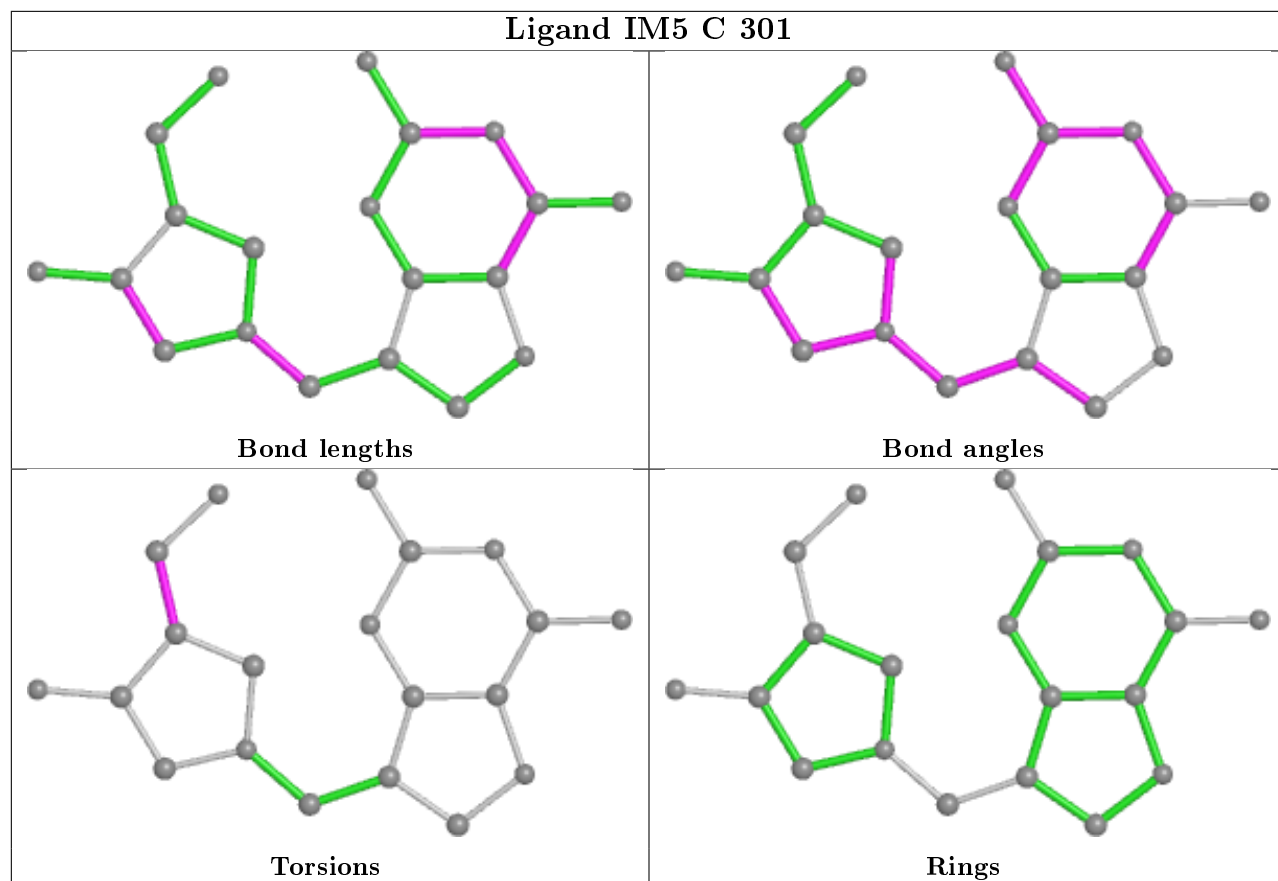| Mol	Chain	Res	Type	Atoms
2	C	301	IM5	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand IM5 A 301

Ligand IM5 C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand IM5 B 301

Bond lengths

Bond angles

Torsions

Rings
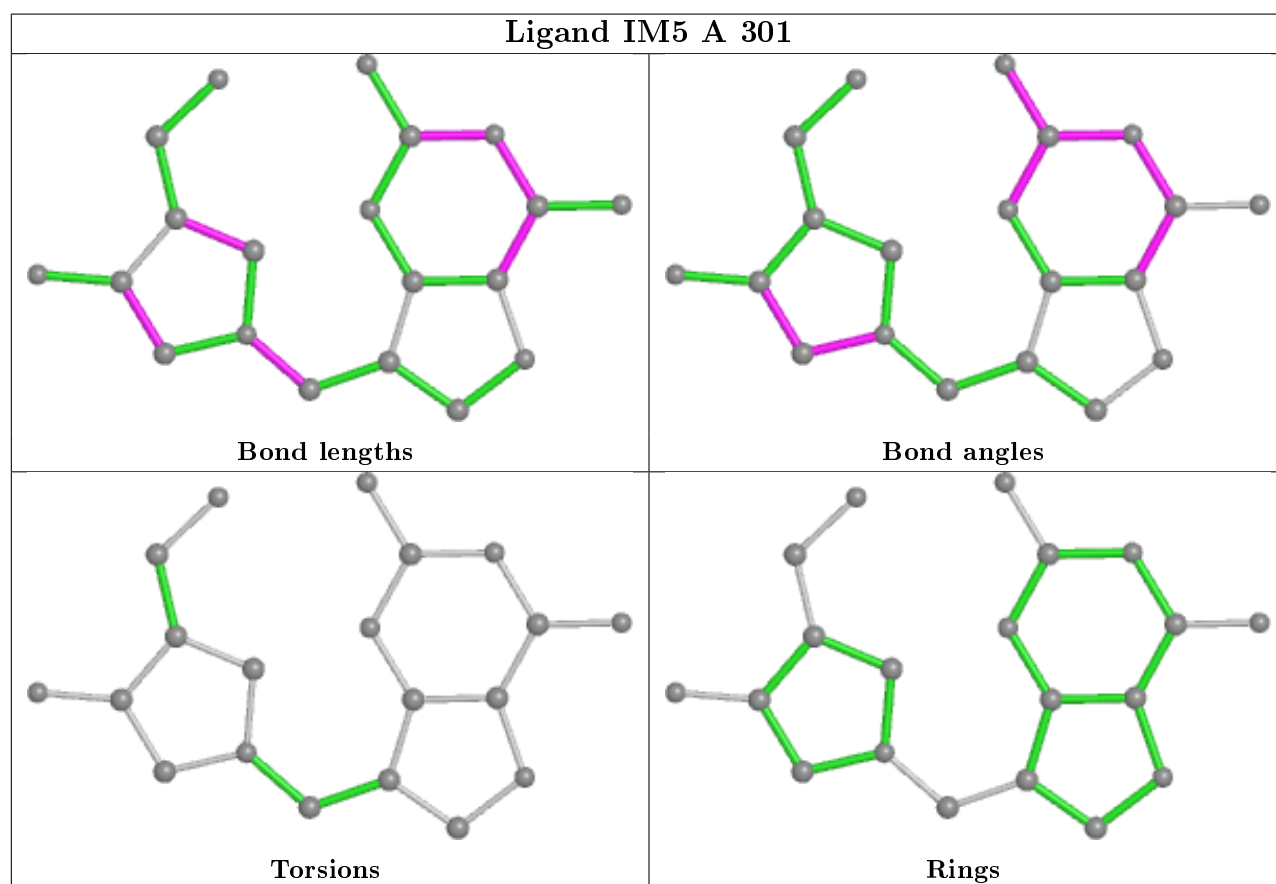
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	282/324 (87%)	0.52	36 (12%)	3	4	22, 34, 62, 120	0
1	B	286/324 (88%)	0.20	15 (5%)	27	30	23, 37, 60, 95	0
1	C	284/324 (87%)	0.54	40 (14%)	2	3	21, 34, 58, 94	0
All	All	852/972 (87%)	0.42	91 (10%)	6	7	21, 35, 62, 120	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	GLY	9.8
1	A	183	GLU	6.9
1	A	184	GLN	6.9
1	A	179	LYS	6.4
1	A	178	TYR	6.1
1	A	180	GLN	5.9
1	C	182	GLY	5.5
1	A	181	MET	5.4
1	C	184	GLN	5.0
1	C	141	PHE	4.6
1	B	184	GLN	4.5
1	C	7	TYR	4.3
1	B	183	GLU	4.3
1	C	138	LEU	4.2
1	A	195	VAL	4.0
1	B	287	LYS	4.0
1	C	222	VAL	4.0
1	A	196	ALA	4.0
1	B	141	PHE	4.0
1	C	142[A]	SER	3.8
1	A	185	ARG	3.7
1	B	3	ASN	3.7
1	B	252	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	4	GLY	3.6
1	A	75	GLY	3.5
1	C	139	PRO	3.5
1	C	143	GLY	3.4
1	B	142[A]	SER	3.4
1	C	195	VAL	3.2
1	C	14	ALA	3.1
1	A	138	LEU	3.1
1	C	15	GLU	3.1
1	A	219	MET	3.1
1	C	16	TYR	3.0
1	A	286	ASP	2.9
1	C	193	VAL	2.9
1	B	250	GLU	2.9
1	C	273	GLN	2.8
1	A	176	SER	2.8
1	A	93	LEU	2.7
1	C	18	LEU	2.7
1	C	226	ILE	2.7
1	A	186	GLU	2.7
1	A	4	GLY	2.7
1	C	93	LEU	2.7
1	B	6	THR	2.7
1	C	194	MET	2.7
1	A	172	GLN	2.7
1	A	142[A]	SER	2.7
1	C	136	ILE	2.6
1	A	88	TYR	2.6
1	C	192	TYR	2.6
1	C	196	ALA	2.5
1	A	139	PRO	2.5
1	B	182	GLY	2.5
1	A	87	MET	2.5
1	A	250	GLU	2.5
1	A	222	VAL	2.5
1	C	147	LEU	2.5
1	A	194	MET	2.4
1	B	58	ARG	2.4
1	C	179	LYS	2.4
1	B	288	ALA	2.4
1	C	140	GLY	2.4
1	B	123	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	287	LYS	2.4
1	A	198	PRO	2.3
1	A	200	PHE	2.3
1	C	178	TYR	2.3
1	A	252	LEU	2.3
1	A	141	PHE	2.3
1	C	223	PRO	2.3
1	A	269	GLN	2.3
1	C	8	GLU	2.2
1	A	175	LEU	2.2
1	A	168	ARG	2.2
1	C	145	ASN	2.2
1	C	219	MET	2.2
1	C	12	ASN	2.1
1	C	11	LYS	2.1
1	C	225	VAL	2.1
1	A	96	VAL	2.1
1	A	217	VAL	2.1
1	C	227	VAL	2.1
1	B	186	GLU	2.1
1	C	221	THR	2.1
1	C	19[A]	SER	2.1
1	A	197	GLY	2.1
1	C	137	ASN	2.1
1	C	58	ARG	2.0
1	C	269	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

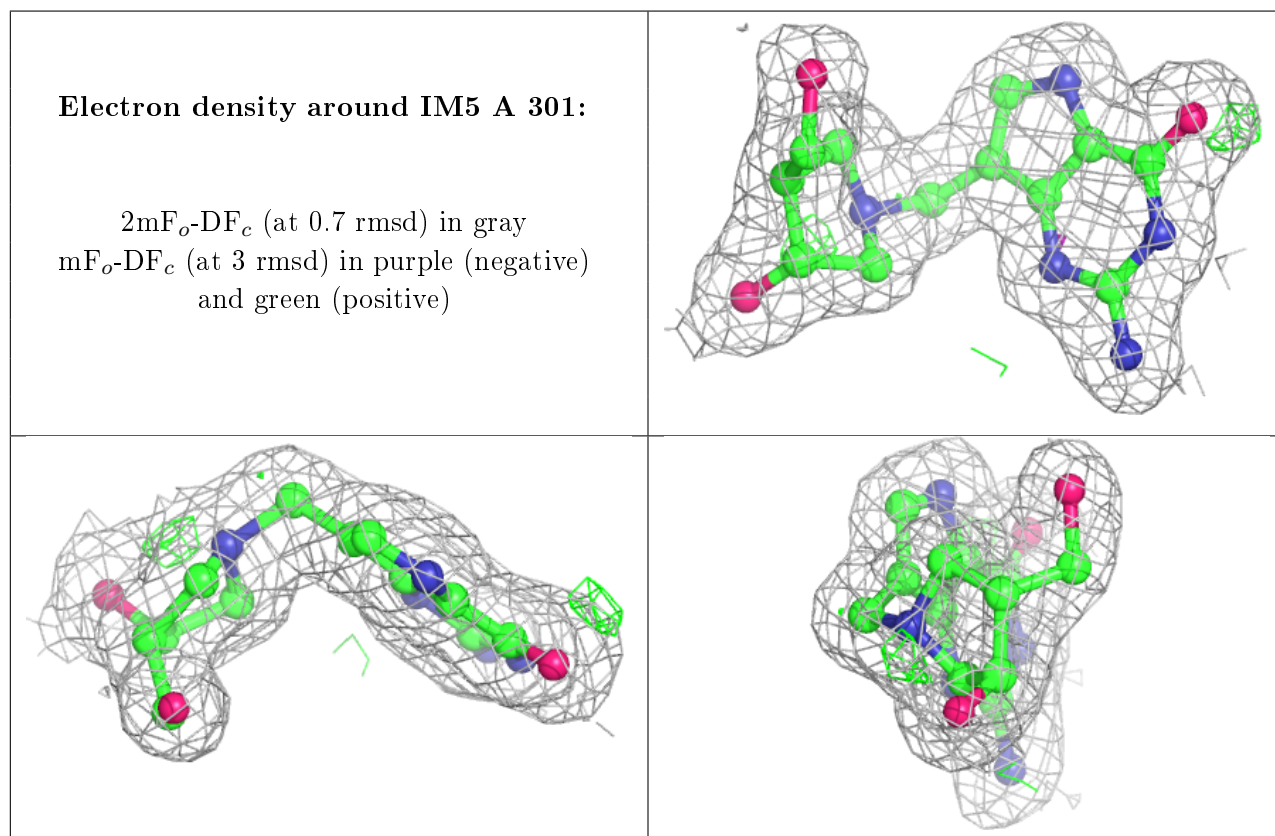| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	FT6	A	257	15/16	0.85	0.13	37,51,59,66	0
1	FT6	C	257	15/16	0.91	0.09	27,36,42,53	0
1	FT6	B	257	15/16	0.92	0.14	33,43,51,55	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
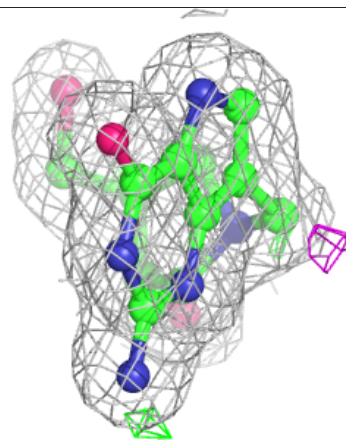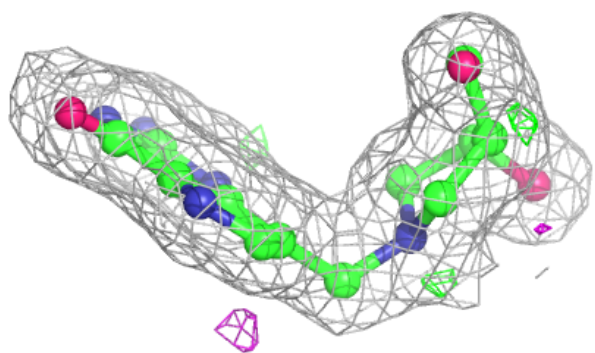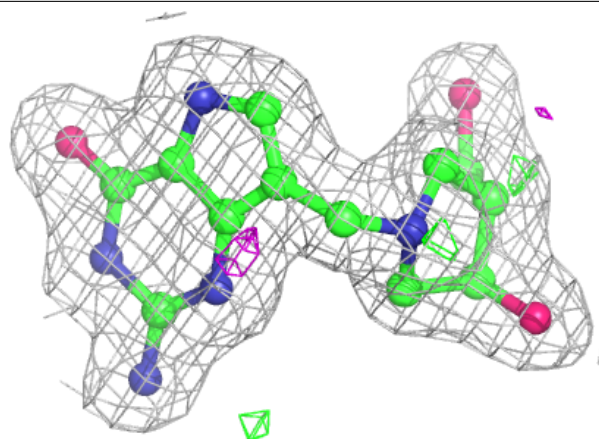
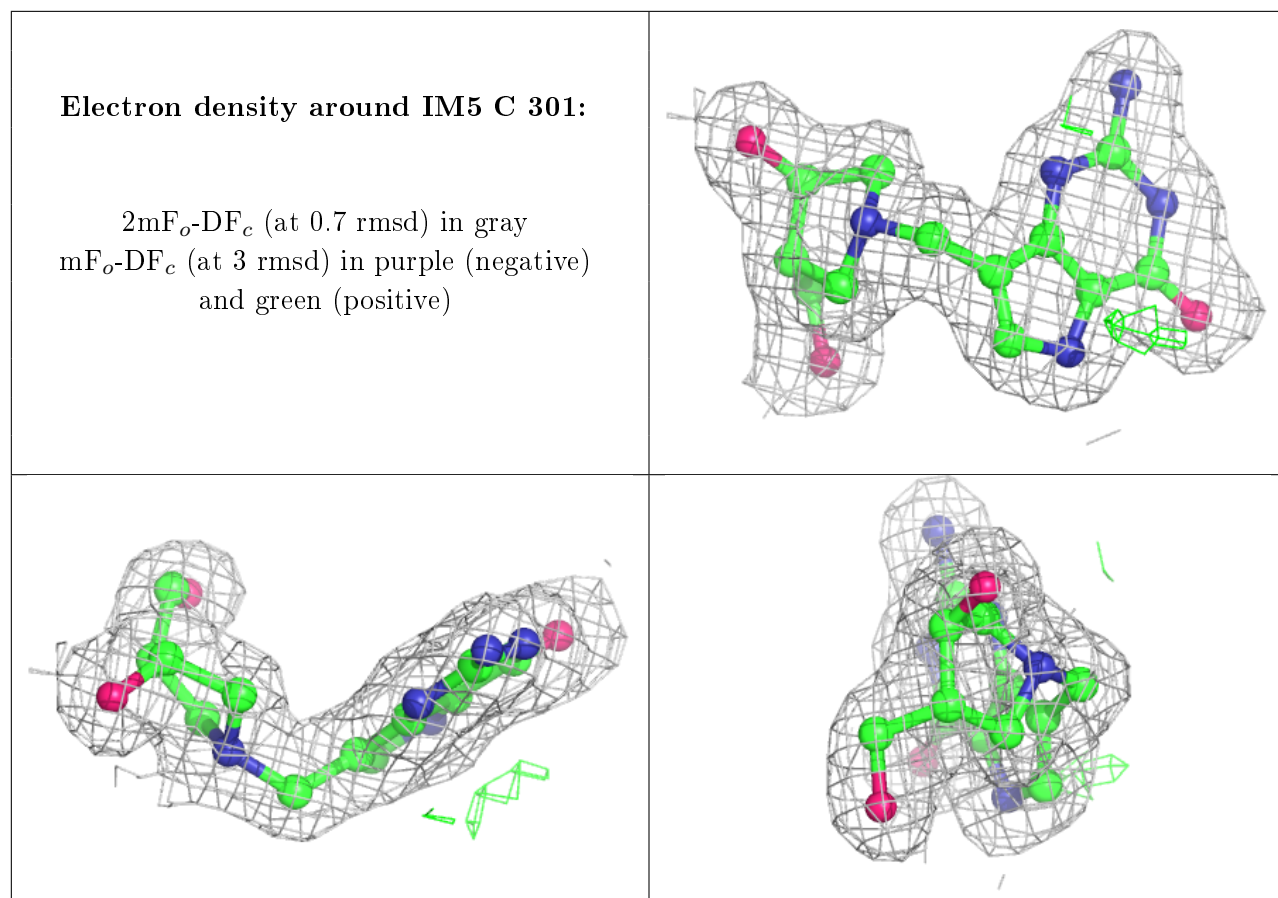| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IM5	A	301	20/20	0.94	0.15	25,26,29,32	0
2	IM5	B	301	20/20	0.97	0.07	22,26,29,32	0
2	IM5	C	301	20/20	0.98	0.12	22,23,26,29	0
3	PO4	B	302	5/5	0.98	0.08	25,26,27,27	0
3	PO4	C	302	5/5	0.99	0.11	23,24,25,25	0
3	PO4	A	302	5/5	0.99	0.12	26,26,27,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around IM5 A 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around IM5 B 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around IM5 C 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.